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Multivariate analysis of energy dispersive X-ray diffraction data for the detection of illicit drugs in border control

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Abstract

A system using energy dispersive X-ray diffraction has been tested to detect the presence of illicit drugs concealed within parcels typical of those which are imported into the UK via postal and courier services. The system was used to record diffraction data from calibration samples of diamorphine (heroin) and common cutting agents and a partial least squares regression model was established between diamorphine concentration and diffraction spectra. Parcels containing various crystalline and amorphous materials, including diamorphine, were then scanned to obtain multiple localised diffraction spectra and to form a hyperspectral image. The calibration model was used for the prediction of diamorphine concentration throughout the volume of parcels and enabled the presence and location of diamorphine to be determined from the visual inspection of concentration maps. This research demonstrates for the first time the potential of an EDXRD system to generate continuous hyperspectral images of real parcels from volume scanning in security applications and introduces the opportunity to explore hyperspectral image analysis in chemical and material identification. However, more work must be done to make the system ready for implementation in border control operations by bringing down the procedure time to operational requirements and by proving the system's portability.

Keywords: X-ray diffraction, Multivariate analysis, Border control, Illicit drugs, Drug detection

Background

A major threat to UK security in recent years has been the importation of illicit drugs via routes such as the postal system and courier services (Coleman 2011; Dhani 2014). The UK Border Force is responsible for ensuring that imported parcels are free from illegal items such as illicit drugs, firearms, explosives and dangerous chemicals before they can be allowed into the country. Manual searching of parcels deemed suspicious on external visual inspection may be time consuming, subject to significant error, and risks damage to the handled parcels. There is therefore a motivation for the development of an automated and non-destructive method to investigate the contents of parcels before they are selected for manual examination (Drakos 2015). The need for the development of efficient and relocatable scanners has been expressed by both the European Commission (Magnusson 2003; Lipoti 2003; Rothschild 2003) and by previous research in the field (Cook et al. 2007, 2009; Griffiths 2008; Koutalonis 2009; Pani 2009). In the interests of efficiency and to minimise disruption through false-positive results, the UK Border Force requires that the duration of initial screening does not exceed 5 min per parcel and be capable of detecting illicit drugs at a minimum threshold of 40% drug purity.

Cocaine and diamorphine are both class A drugs, classified according to the Misuse of Drugs Act 1971 (MDA), and are the most commonly seized drugs in the UK with approximately 17,000 and 8500 seizures in 2013/2014, respectively (Dhani 2014). Due to the limited availability of cocaine during the experimental phase of the research, this study focuses on the detection of diamorphine.

Energy dispersive X-ray diffraction (EDXRD) is a non-destructive technology which has previously been

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employed in laboratory settings to scan the contents of letters, parcels, boxes, suitcases and palletised goods to identify illicit drugs and explosive materials (Luggar 1995, 1996a, b; Strecker 1993; Speller 1996, 2001). A portable prototype for use in border control, which operates at room temperature, has been developed during the experimental phase to scan large volumes containing amorphous and crystalline materials (Drakos 2015). The objective of this research is to test the system for its feasibility in detecting materials of interest using EDXRD in the context of fast-parcel screening. The study predicts the presence of seized diamorphine, which had subsequently been concealed in parcels typical of those encountered at border control. The research introduces continuous hyperspectral imaging of parcel cross sections and employs the well-established partial least squares regression method on the resulting hypercubes to predict illicit drug concentration locally through the parcel volume. The results of this study motivate further research using spectroscopic image analysis and chemometric methods to advance the exploration and prediction methodology from hyperspectral diffraction images in security applications (Amigo et al. 2015). The research presented here is a proof of concept of full-volume parcel screening and future work is required to bring down the current 30 min procedure time to meet the time constraints set by UK Border Force. To this end, data acquisition times may be reduced by increasing the X-ray flux of the system, or through image analysis performed on lower resolution diffraction images.

X-ray diffraction

Conventional X-ray transmission imaging systems used in border control provide information about the object density and the effective atomic number of concealed materials; this is useful in the visual identification of materials with high atomic numbers such as metallic items which have higher transmission image contrast and have distinguishable morphology. They cannot however be readily used for the identification of materials with low atomic numbers, such as drugs and explosives where the contrast is low and the morphology is not distinct. X-ray diffraction is an appropriate technique for material characterisation as it produces a diffraction pattern which is a unique fingerprint of substances, representing their chemical composition. Diffraction occurs when X-rays are scattered from the molecular planes within a material following which they constructively interfere. The wavelengths (λ) of the diffracted X-rays and the angles through which they are diffracted (θ) are related to the molecular planar spacings (d) of the material by Bragg's law:

$$n\lambda = 2d \sin\theta \tag{1}$$

where the energy (E) of a scattered photon is related to its wavelength by the following relation:

$$E = \frac{hc}{\lambda} \tag{2}$$

where h is Planck's constant and c is the speed of light in a vacuum. All crystalline materials have a unique set of planar spacings (d) and thus the distribution of measured photon energies and corresponding diffraction angles describe uniquely the chemical composition of the crystalline sample. Two types of diffraction patterns can be obtained by measuring the intensity distribution of scattered photons:

- Varying the angle of detection using a monochromatic X-ray source—a method known as angular dispersive X-ray diffraction (ADXRD);
- Using a polychromatic X-ray source and detecting scatter at a fixed angle—a method known as energy dispersive X-ray diffraction (EDXRD).

ADXRD is a well-established technique for producing high quality diffraction patterns using a synchrotron X-ray source in combination with a high resolution area-detector (Harding and Schreiber 1999; Bohndiek 2008). However, the photon throughput from ADXRD techniques is typically low and leads to long data acquisition times. The beam energies from such monochromatic sources are low (<10 keV) and due to attenuation effects at low beam energies the penetration depth is insufficient for scanning the volume of a parcel. Furthermore, such a diffractometer contains highly sensitive moving parts to detect X-rays at varying angles thus limiting a system's portability. It is for these reasons a system using ADXRD has not been developed for parcel screening.

In EDXRD, a collimated energy-resolving detector at a fixed angle is used to measure forward scatter events from a polychromatic source of X-rays, as shown in Fig. 1. Diffraction from molecular planes alters the incident spectrum forming a diffraction profile of the materials as measured by the detector. Focusing on low angle (3°–7°) forward scatter, where photons are scattered coherently, produces an intensity distribution containing information on both the chemical composition and the crystallinity (Cook 2008). Furthermore, the scatter fields correspond to a well-defined volume within the material, which enables volume imaging, improves localisation and has the potential to increase the detection rate by increasing the specificity of a system (Luggar and Gilboy 1999).

Using multivariate analysis and a training set of known material mixes, a regression model can be built for

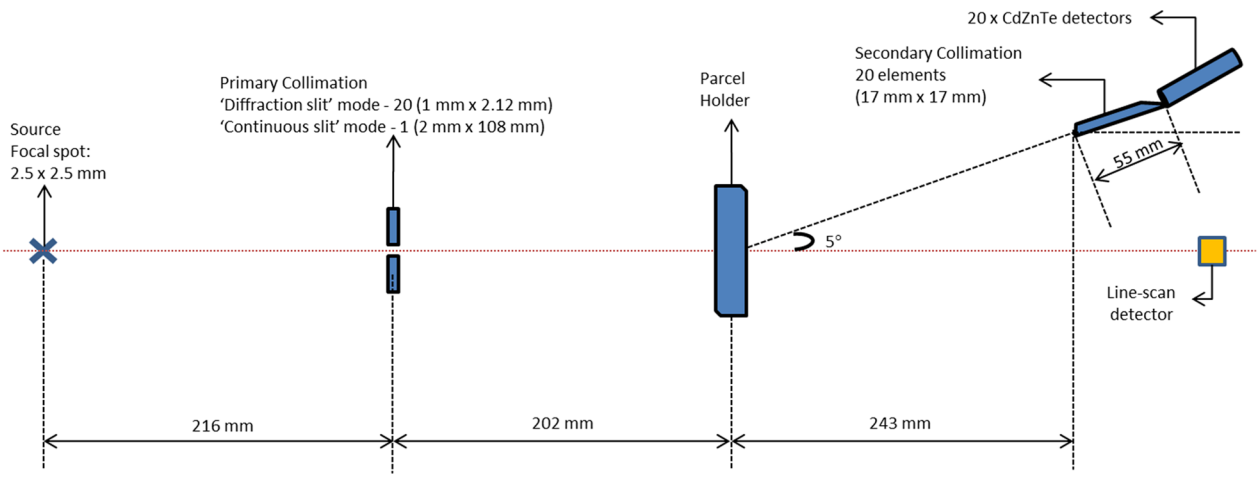

Fig. 1 EDXRD schematic. Schematic showing the EDXRD setup. The X-ray source is collimated and focused into a scattering volume at which the parcel or calibration sample is placed. Diffracted X-rays are detected by 20 CdZnTe detectors each positioned at a fixed angle of 5°

predicting the quantity of illicit drugs in an 'unknown' sample (Luggar 1996b; Speller 2001). It has been reported that by implementing EDXRD, even at short acquisition times leading to a total of 200 photon counts, a system can still distinguish between drugs, explosives and other arbitrary objects using the multivariate analysis technique (Speller 2001). More specifically, in the field of airport security, EDXRD has been suggested for the detection of illicit materials inside suitcases (explosives) and parcels (drugs) (Strecker 1993; Luggar 1995, 1996a, b; Speller 1996, 2001). Research has been extended to the classification and identification of drugs (Cook et al. 2007, 2009; Cook 2008; Griffiths 2008; Koutalonis 2009; Pani 2009) in an environment in which the samples are concealed within a container. With scatter photon throughput approximately three orders of magnitude greater than ADXRD (Harding and Schreiber 1999), EDXRD techniques lead to reduced measurement times for real-time practical applications, such as fast-parcel systems (Drakos 2015).

Methods

System specification

A tungsten target (W) X-ray source tube (Monoblock®, Spellman High Voltage Electronics Corporation) with maximum output potential settings of 140 kV and 5 mA was used for all the experiments. The source had an inherent filtration of 0.8 mm Be and 1.5 mm glass. Additional filtration of 12–15 mm (max) oil (Shell Diala A), 0.41 mm Al and 0.04 mm Cu was included on the X-ray tube casing and the source had a nominal focal spot size of 2.5 × 2.5 mm. The scattered photons were detected at a nominal angle of 5° using twenty off-the-shelf CdZnTe detectors with crystal dimensions of 5 × 5 × 5 mm (SPEAR, eV Products) and energy resolution of 6% at 59.6 keV (Drakos 2015). Twenty detectors were used in order to interrogate 20 discrete scatter volumes of 10 × 10 × 10 mm within the parcels simultaneously. High voltage gain amplifiers and multichannel analysers (ORTEC®) were used to retrieve the measured diffraction profile by binning the voltage pulses to one of 512 channels in a format (Maestro, ORTEC®) that could be read

Table 1 The concentrations of diamorphine and cutting agents in the calibration samples

#	Diamorphine concentration (%)	Cutting agent	Concentration (%)
1	100	–	0
2	90	Caffeine	10
3	70	Caffeine	30
4	50	Caffeine	50
5	90	Lidocaine	10
6	80	Lidocaine	20
7	60	Lidocaine	40
8	50	Lidocaine	50
9	90	Paracetamol	10
10	80	Paracetamol	20
11	70	Paracetamol	30
12	60	Paracetamol	40
13	50	Paracetamol	50
14	90	Mannitol	10
15	80	Mannitol	20
16	70	Mannitol	30
17	60	Mannitol	40
18	50	Mannitol	50

by both The Unscrambler (v.9.5, CAMO) and MATLAB® (v.2014b, MathWorks) software packages.

The incident beam was collimated by a purpose-built 10 mm thick lead structure operating in two modes: (i) transmission mode with dimensions 2 mm wide x 108 mm tall; and (ii) diffraction mode with 20 slits (corresponding to the 20 individual CdZnTe detectors) each with dimensions of 1 mm wide x 2.12 mm tall and configured as depicted in Fig. 1 (Drakos 2015). The use of a primary collimator ensures that the incident X-ray beam is collimated to a narrow beam. The collimation of the scattered photons was provided by a set of 20 soller-slit collimators of 17 mm width, 17 mm height and 55 mm depth placed at a nominal scattering angle of 5° from the scattering centre. These collimators could be interchanged such that the slits were either perpendicular or parallel to the X-ray beam field. Lastly, a line-scan X-ray detector (C9750-10FC, Hamamatsu) was chosen to capture transmission images of interrogated objects.

Calibration data

The calibration library was comprised of 18 samples: 1 sample of pure diamorphine and 17 binary samples of pharmaceutical grade diamorphine HCL mixed with cutting agents. The most common cutting agents used with illicit diamorphine are caffeine and paracetamol and were used for the binary mixtures of the calibration samples. Additionally, lidocaine and mannitol were also included in the design as the former is a common active pharmaceutical ingredient and the latter is used commonly for increasing the volume of the product (Coomber 1997; Gomez and Rodriguez 1989; Kaa 1994). All calibration samples and their concentrations of diamorphine and cutting agent are given in Table 1. The library was prepared by affiliates of the Centre for Applied Science and Technology (one of the main science and technology units of the UK Home Office) in 2 mm thick by 70 mm long cylindrical Perspex tubes of 26 mm internal diameter, amounting to a total mass of 16 g in each sample. The

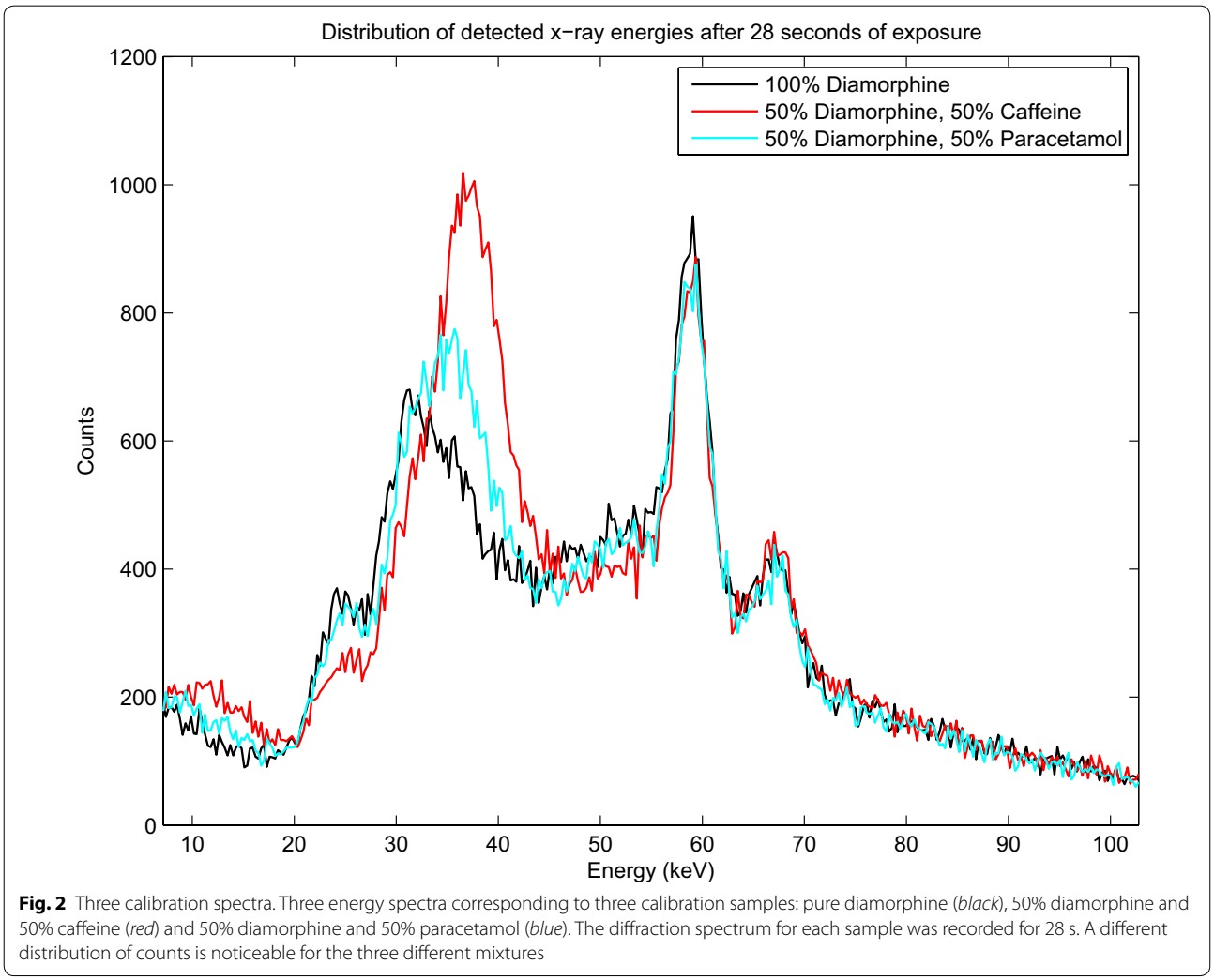

Fig. 2 Three calibration spectra. Three energy spectra corresponding to three calibration samples: pure diamorphine (*black*), 50% diamorphine and 50% caffeine (*red*) and 50% diamorphine and 50% paracetamol (*blue*). The diffraction spectrum for each sample was recorded for 28 s. A different distribution of counts is noticeable for the three different mixtures

tubes were sealed with Kapton® polyamide film to minimise the attenuation of photons. The tubes were placed on the sample holder and their diffraction profiles were acquired under the source's maximum settings, 140 kVp and a constant current at 5 mA, using the middle diffraction beam and scattering cell slits arranged perpendicular to the scattering plane (Drakos 2015). Diffraction profiles were recorded for 28 s for all samples. An R-quality factor optimisation study was carried out on the calibration samples to obtain the optimum recording time for diffraction profiles using the system. This recording time was selected according to the corresponding signal-to-noise ratio (SNR) and the minimum interrogation time such that the error was 5% or less (Drakos 2015). The scatter from an empty sealed tube was measured and its effects subtracted from all subsequent spectra in the calculations.

Modelling framework

The energy distribution of X-ray photons detected during a scan form an intensity spectrum which is recorded by the multichannel analyser. The location and distribution of peaks in the recorded spectra correspond to the molecular planar spacings of the samples' chemical components and thus describe uniquely the chemical composition of the sample. Figure 2 shows the distribution of X-ray photon energies for three calibration samples: one of pure diamorphine and the other two comprising 50% diamorphine and 50% caffeine, and 50% diamorphine and 50% paracetamol for scans with duration of 28 s. The spectra in Fig. 2 show between-sample variation for different mixtures of diamorphine and cutting agents. A calibration model regresses the concentration of diamorphine in the samples against the counts measured in the energy channels in order to model the variation in diamorphine concentration between spectra.

The spectral matrix X is formed of 18 rows corresponding to the calibration samples and 350 columns corresponding to the energy channels across which between-sample variation was observed. The spectral data matrix X can be assumed to be linearly and additively related to the concentrations of chemical components according to Beer–Lambert's law:

$$X = YA \tag{3}$$

where Y is the matrix of concentrations of the chemical components and A is the matrix of standardised diffraction contributions to each energy channel from each chemical component. When investigating volumes of unknown components, the spectral data is recorded and the concentrations are unknown and are to be predicted. An inverse calibration model is built to regress the concentrations of diamorphine against spectral data:

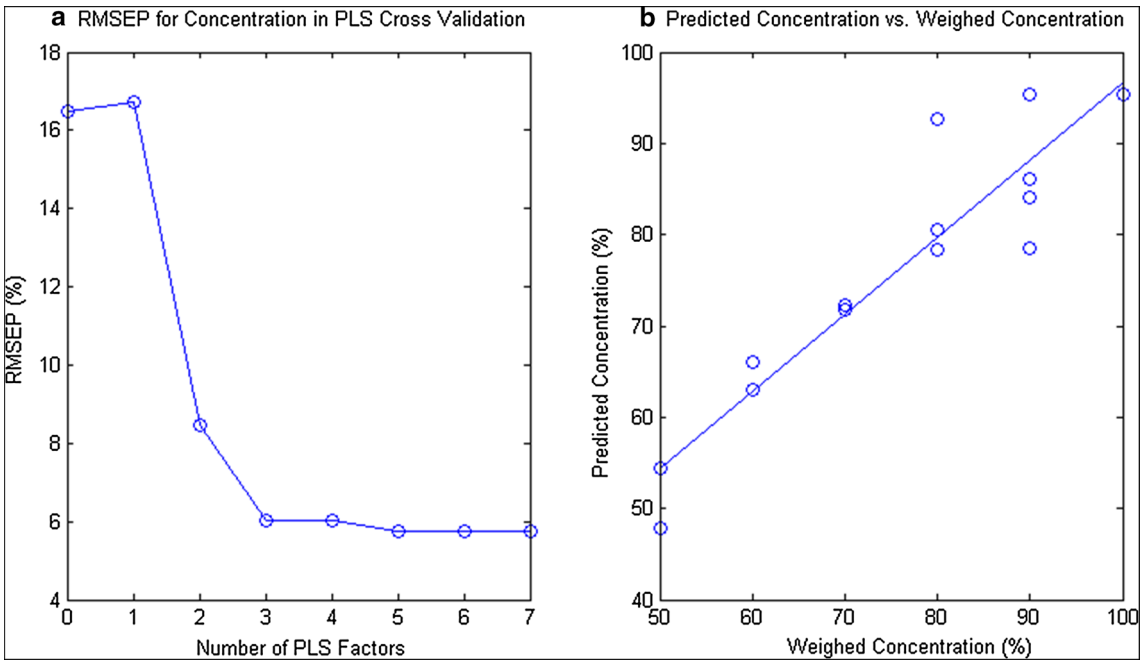

Fig. 3 Calibration results. **a** RMSECV for PLS calibration models of diamorphine concentration with a minimum at 5 factors and RMSECV of 5.8%. **b** Predicted diamorphine concentrations from 5 factor PLS model vs. weighed concentrations

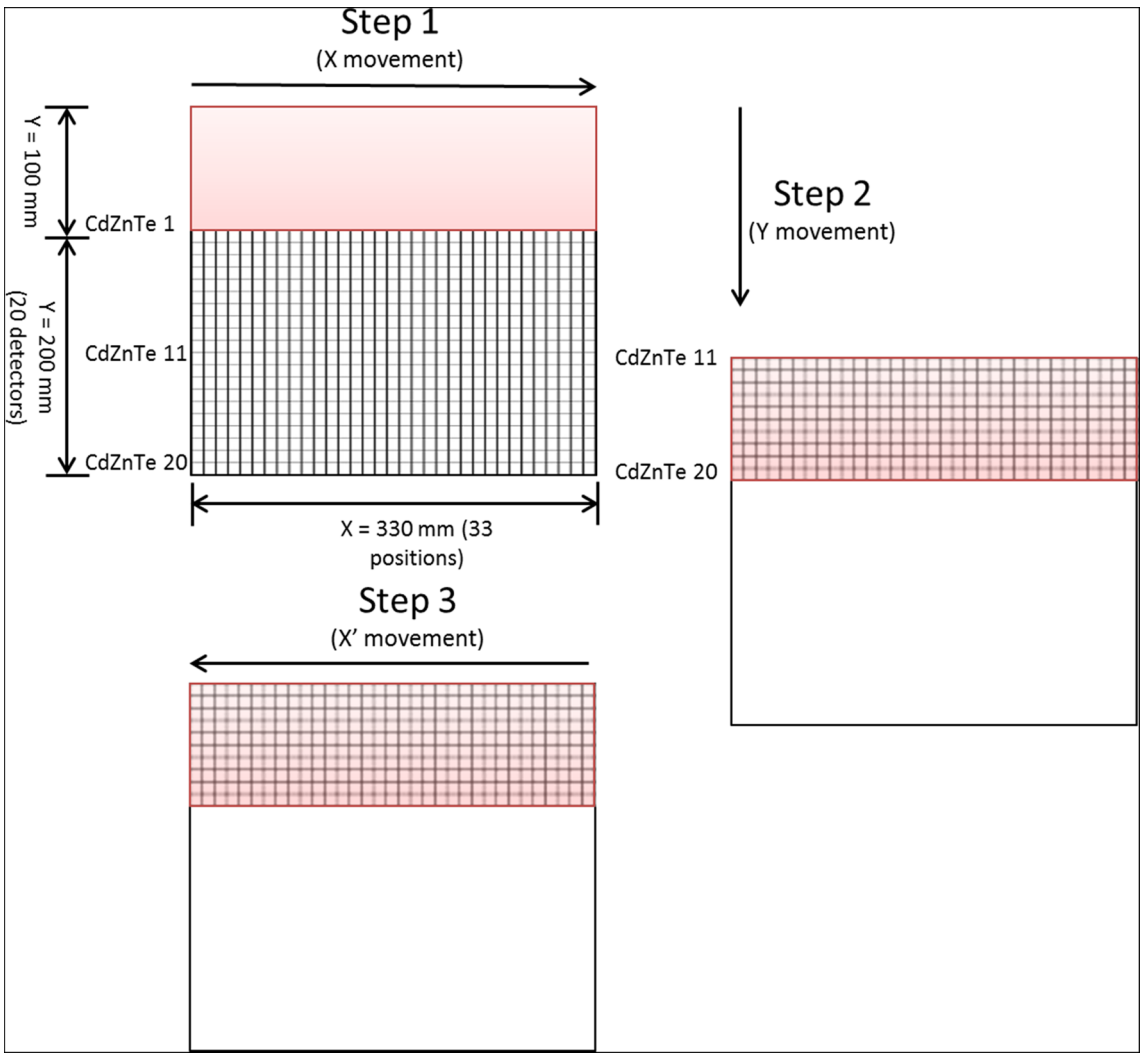

Fig. 4 Parcel scanning geometry. In Step 1 of parcel scanning, 20 detectors simultaneously record diffraction data from the lower region of the parcel from the *left hand side* to the *right* as the parcel is translated. The parcel is then translated downwards in Step 2. Finally in Step 3 the detectors record diffraction data on the remaining parcel region from the opposite side (*right hand side* to *left*)

$$y = Xb + E \tag{4}$$

where y is the concentration vector of diamorphine, X is the matrix of diffracted photon counts, b is the regression vector and E is the error in the model. Due to the high collinearity of the spectral variables in X, partial least squares (PLS) regression was used to calculate the regression vector b by finding a small number of uncorrelated latent factors from the spectral variables that maximise the covariance between the concentration vector y and the spectral matrix X (Martens and Naes 1992). To determine the optimum number of PLS factors, a leave-one-out cross validation was carried out on the calibration set for different numbers of PLS factors. The number of PLS factors which minimised the root mean squared error of cross validation (RMSECV) was found to be 5 as shown in Fig. 3a. The number of PLS factors chosen for the calibration model was 5 factors and the RMSECV for the calibration model was 5.8%. The predicted concentrations of diamorphine using the 5 factor PLS calibration model are plotted against the weighed concentrations in Fig. 3b.

Parcel scanning

For parcel scanning, the parcel is divided into volume elements with cross-sectional area perpendicular to the incident beam of 10 mm × 10 mm, and each is scanned for 28 s to record localised diffraction spectra throughout

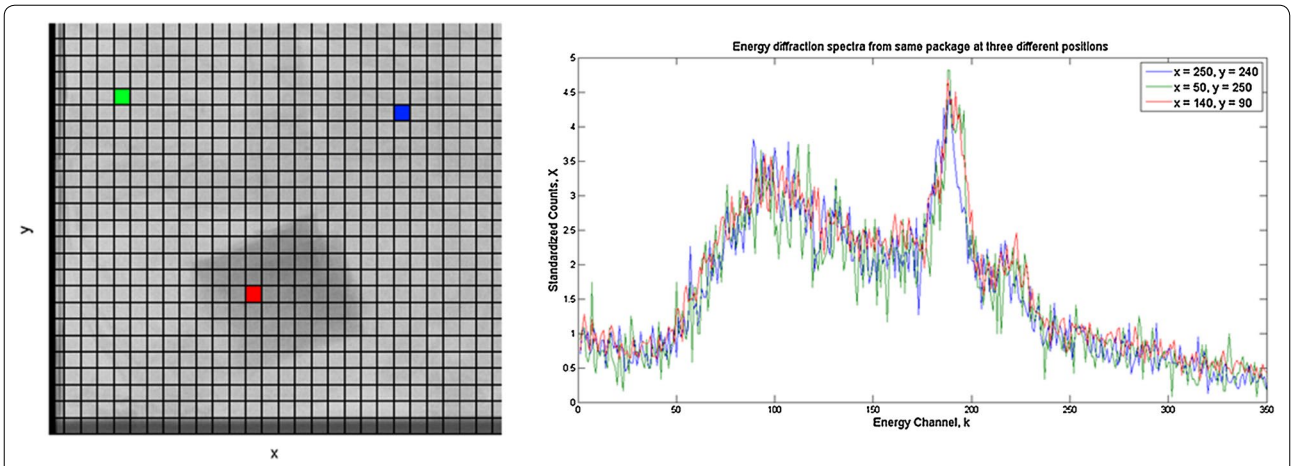

Fig. 5 Parcel scanning schematic. Three selected volume elements (*left*) and their corresponding standardised diffraction spectra (*right*) from a scanned parcel. The concentration of diamorphine in each volume is predicted via the regression calibration model in order to form a concentration map of diamorphine

the volume. The 20 beam collimators and corresponding CdZnTe detectors enabled 20 volume elements to be scanned simultaneously. Initially, columns of the lowest 20 volume elements of the object are scanned consecutively. Multiple sweeps are made across objects where the object is larger than the X-ray beam as demonstrated in Fig. 4. Figure 5 shows three selected volume elements for a sample parcel and the corresponding diffraction spectra for each.

The predicted concentration vector $\hat{y}$ for the volume elements is calculated using the corresponding measured spectra X according to the prediction model:

$$\hat{y} = X\hat{b} \tag{5}$$

where $\hat{b}$ is the calculated regression vector from the calibration model. Following calculating the predicted diamorphine concentration vector, the vector is refolded into a two-dimensional concentration map for visual inspection of the parcel for drug detection.

Results and discussion

Three parcels were scanned and analysed to test the system with their contents given in Table 2. The parcel contents were chosen to test the capability of the system to identify regions containing diamorphine (Parcel 1), to disregard regions containing crystalline materials other than diamorphine (Parcel 2) and to be able to identify diamorphine in parcels containing the drug in several locations and with reflective surfaces (Parcel 3).

Figure 6 shows the results of the diamorphine prediction on the three parcels along with their corresponding transmission images. A threshold of 40% diamorphine concentration has been set on the concentration maps in accordance with the UK Border Force's requirement to reduce false positive results.

The concentration map of Parcel 1 (Fig. 6a) identifies the sample of diamorphine at 73% purity which can be seen in the transmission image in the lower central area of the image. Decreased transmission intensity is also observable in the lower right region of the image corresponding to a book. The concentration map correctly identifies the diamorphine sample and disregards the book and all other materials within the parcel leading to a true positive result.

Parcel 2 (Fig. 6b) contains textiles and a sample of the crystalline material sodium bicarbonate. From the transmission image the heavily scattering region in the centre of the image corresponds to the location of sodium bicarbonate. The concentration map does not predict diamorphine in this region and thus demonstrates a true negative result for crystalline materials. The rows corresponding to $y = 30$–50, 230–250 regard

Table 2 The contents and results of the three analysed parcels to test for diamorphine

#	Contents	Result
1	Book, textiles, lead gloves and sample of 73% diamorphine and unknown cutting agents	True positive
2	Textiles and sodium bicarbonate	True negative
3	Sample of 69% diamorphine placed in textile samples, sample of 69% diamorphine stuffed within soft toys, and three DVDs	True positive

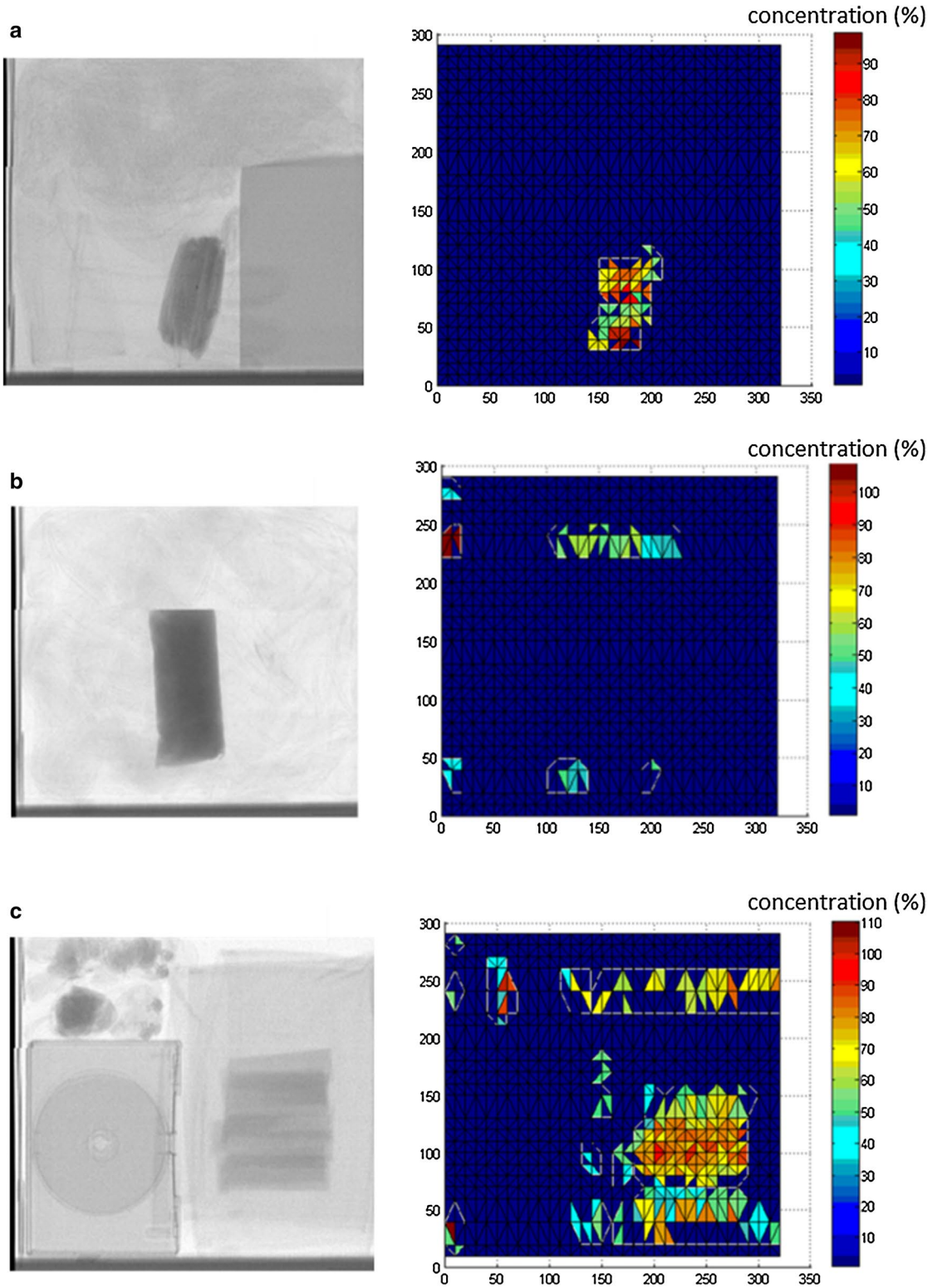

Fig. 6 Parcel prediction concentration maps. Transmission images (*left*) and diamorphine concentration maps (*right*) of three analysed parcels: **a** Parcel 1: 73% purity diamorphine sample with unknown cutting agent. **b** Parcel 2: pure sample of sodium bicarbonate. **c** Parcel 3: 69% purity diamorphine sample with unknown cutting agents located middle right and top left, and 3 DVDs located bottom left

diffraction profiles recorded by the same three CdZnTe detectors known to be malfunctioning during the experiment thus leading to dead pixels and spikes within the recorded spectra. These rows have been omitted from subsequent analysis. The faults in these detectors were due to defects in their electrical contacts causing unstable bias voltage (LeClair 2006; Knoll 2010).

Parcel 3 (Fig. 6c) contains samples of diamorphine at 69% purity found in two locations. A large sample was wrapped in textiles and can be observed in the central right region of the transmission image. The concentration map identifies diamorphine correctly within this region. A smaller sample of diamorphine concealed within a soft toy is observable in the top left of the transmission image, above the DVD cases. A strong prediction of diamorphine concentration is determined at this location. However, the position of the sample coincides with the malfunctioning detectors, resulting in false positive results in the same rows to the right of the concentration map. The three DVDs observable in the lower left of the tranmission image are not mistakenly identified as diamorphine. The volume elements corresponding to the malfunctioning detectors notwithstanding, this parcel has a true positive result for identifying diamorphine.

Conclusions

The multivariate analysis technique of partial least squares regression has been demonstrated to be capable of identifying the illicit drug diamorphine in parcels containing a variety of crystalline and amorphous materials using the portable EDXRD system described previously (Drakos 2015). In the three parcels investigated the presence or absence of diamorphine could be accurately identified from visual inspection of concentration maps. To fully characterise and assess the sensitivity and specificity of the system the process is to be expanded to 75 parcels. In order to accurately identify diamorphine from parcel diffraction spectra the volume elements were scanned for 28 s leading to a total scanning time per parcel in excess of 30 min. To satisfy the UK Border Force requirements of a maximum scanning time of 5 min, improvements to the system design, signal processing or calibration model are required and will be the focus of future work. Recent methodology developed for the analysis of hyperspectral images will be explored to motivate improvements in drug detection performance (Amigo 2015).

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Authors' contributions
ID set up the portable EDXRD system and took the measurements. ID and PK analysed the data. PK drafted the manuscript. RS is the principal investigator for the project. TF consulted on the statistical analysis. All authors read and approved the final manuscript.

Competing interests
The authors declare that they have no competing interests.

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